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SUPPORTING INFORMATION

Title: Predicting Solubility of Military, Homemade, and Green Explosives in Pure and Saline Water using COSMO-RS

Author(s): S. Alnemrat, J. P. Hooper*

Ref. No.: prep.201300071

Predicting solubility of military, homemade, and green explosives in pure and saline water using COSMO-RS

Sufian Alnemrat and Joseph P. Hooper*

Department of Physics, Naval Postgraduate School, Monterey, California 93943, United States

Table S1. Mass-based concentration of Na^+ and Cl^- ions, ionic strength, and salting-out coefficients at different temperature for all compounds in the training set.

Concentration of Ions	1g salt/100g water	2g salt/100g water	3g salt/100g water	4g salt/100g water	5g salt/100g water	6g salt/100g water		
Ionic Strength (mol/L)	0.179	0.358	0.537	0.716	0.896	1.07		
Salting-out Coefficient (L/mol)								
Temperature (^{0}K)	263	273	283	293	303	313	323	333
2NT	0.20	0.21	0.21	0.22	0.22	0.22	0.23	0.23
3NT	0.22	0.23	0.25	0.26	0.27	0.27	0.28	0.28
4NT	0.21	0.23	0.24	0.25	0.26	0.27	0.28	0.28
24DNT	0.19	0.21	0.23	0.25	0.26	0.27	0.29	0.29
26DNT	0.20	0.22	0.23	0.25	0.26	0.27	0.28	0.29
DNB	0.17	0.19	0.20	0.22	0.23	0.25	0.26	0.27
NB	0.19	0.20	0.21	0.22	0.23	0.24	0.25	0.26
TNB	0.21	0.22	0.24	0.26	0.27	0.28	0.30	0.30
TNT	0.23	0.25	0.27	0.28	0.31	0.31	0.32	0.33
EGDN	0.23	0.24	0.25	0.25	0.26	0.26	0.27	0.27
NG	0.36	0.36	0.36	0.37	0.37	0.38	0.38	0.38
PETN	0.39	0.40	0.41	0.41	0.42	0.43	0.44	0.45
2ADNT	0.15	0.17	0.20	0.22	0.24	0.25	0.27	0.28
4ADNT	0.14	0.17	0.19	0.21	0.23	0.25	0.26	0.27
RDX	0.12	0.15	0.17	0.19	0.20	0.22	0.24	0.25
β-HMX	0.06	0.08	0.10	0.13	0.16	0.19	0.21	0.23
TATB	0.18	0.20	0.22	0.24	0.26	0.27	0.29	0.30
CL-20	0.30	0.32	0.34	0.36	0.38	0.40	0.41	0.42

* Corresponding author.
Email address: jphooper@nps.edu (J.P. Hooper)

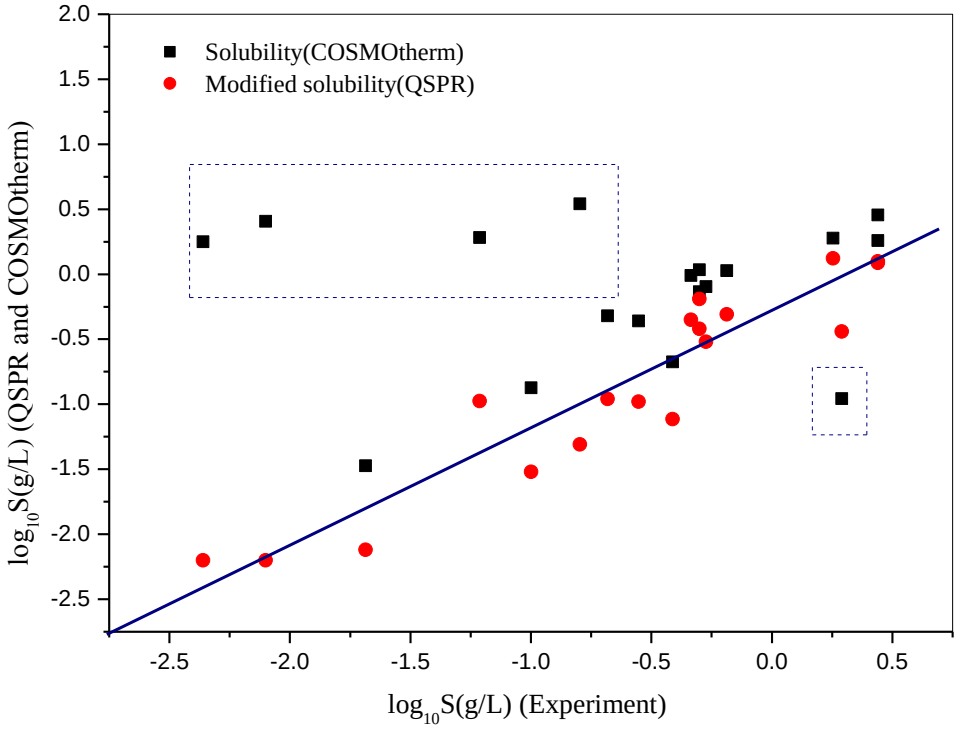

Figure S1. Comparison between direct COSMO-RS predictions and modified calculations using QSPR method for RDX and Cl-20. Points inside boxes show the poor solubility predictions for some important compounds such as RDX, CL-20, and HMX using direct COSMOtherm calculations.

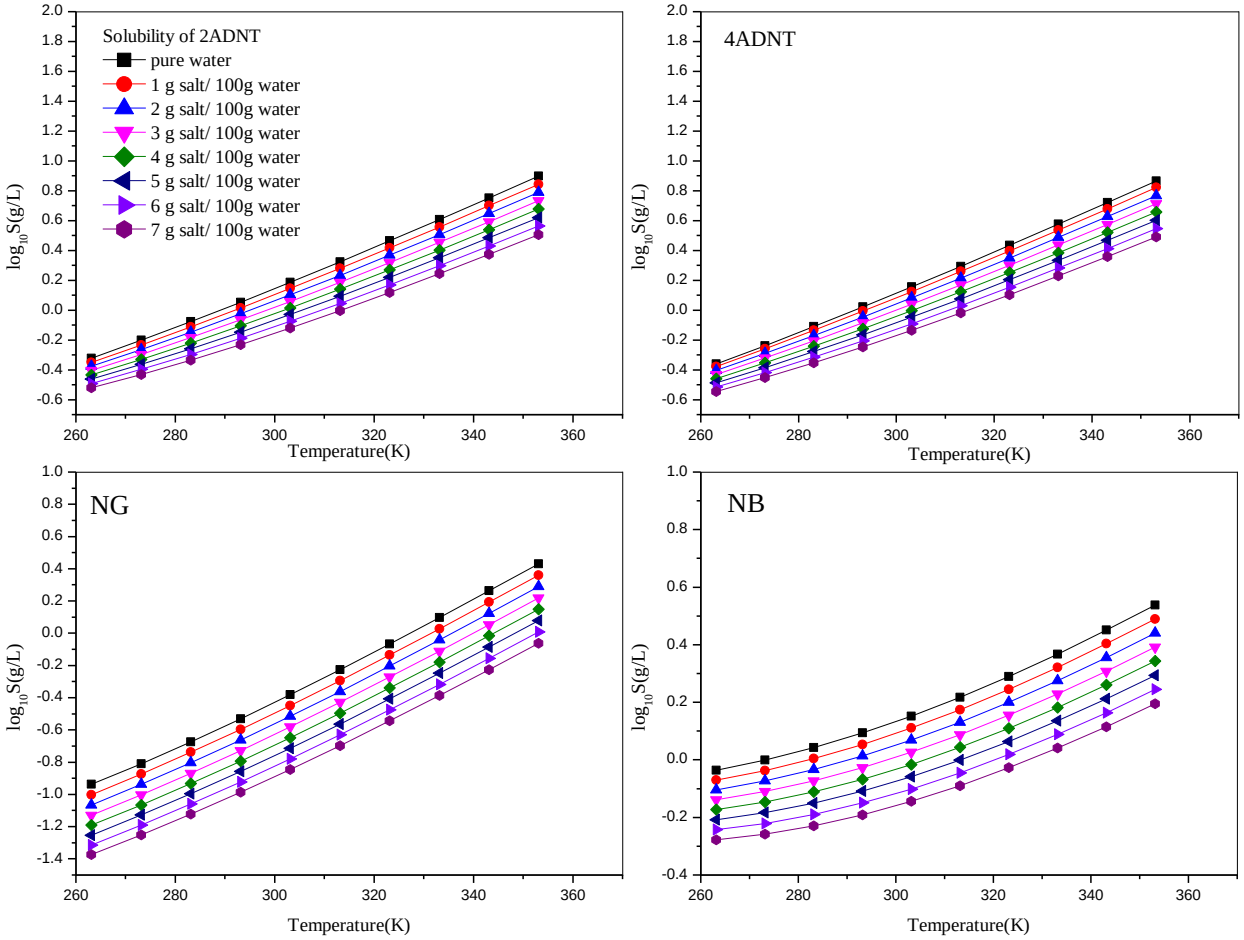

Figure S2. Higher-solubility compounds in the training set as a function of temperature and ionic strength.

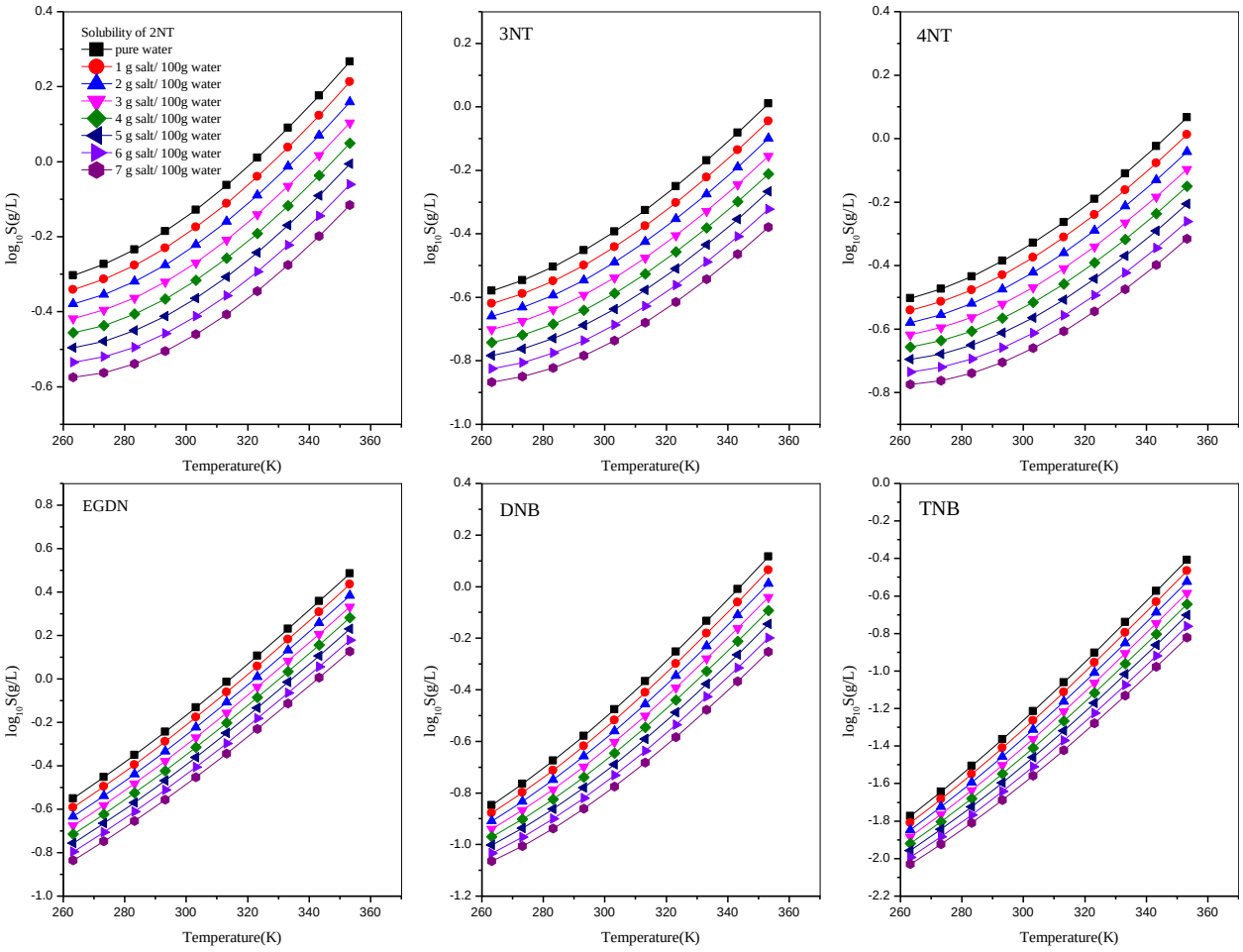

Figure S3. Intermediate-solubility compounds in the training set as a function of temperature and ionic strength.

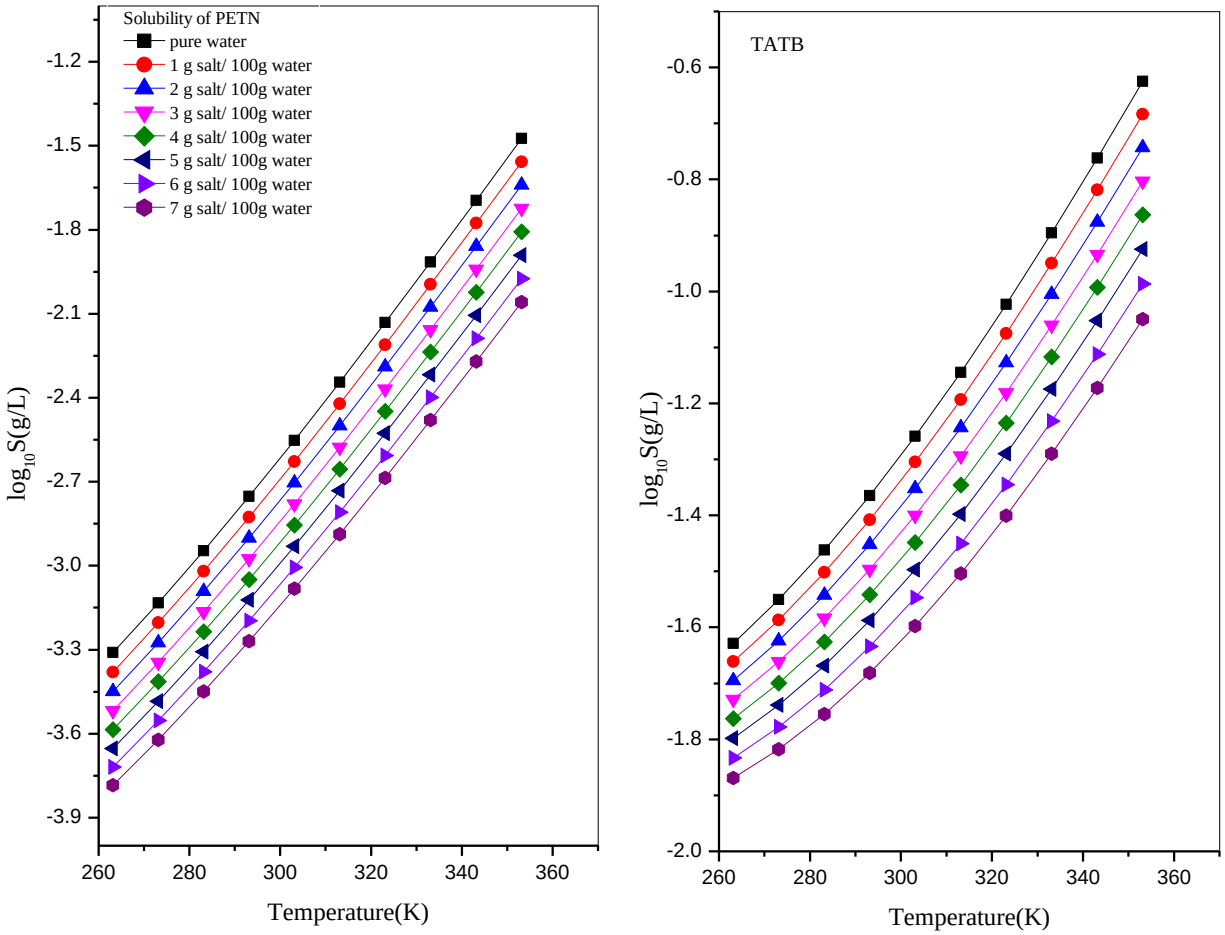

Figure S4. Low-solubility compounds in the training set as a function of temperature and ionic strength.

Table S2. Mass-based concentration of Na^+ and Cl^- ions, ionic strength, and salting-out coefficients at different temperature for all compounds with no experimental data.

Concentration of Ions	1g salt/100g water	2g salt/100g water	3g salt/100g water	4g salt/100g water	5g salt/100g water	6g salt/100g water
Ionic Strength (mol/L)	0.179	0.358	0.537	0.716	0.896	1.07

Salting-out/in Coefficient (L/mol)								
Temperature (^{0}K)	263	273	283	293	303	313	323	333
FOX7	0.16	0.17	0.18	0.19	0.19	0.20	0.21	0.22
DDNP	0.08	0.10	0.13	0.16	0.18	0.20	0.22	0.24
DMNB	0.22	0.24	0.25	0.26	0.27	0.29	0.30	0.30
NQ	-0.09	-0.07	-0.05	-0.02	-0.01	-0.006	0.007	0.018
TATP	0.41	0.41	0.42	0.42	0.42	0.43	0.43	0.44
TNA	0.14	0.16	0.19	0.21	0.23	0.25	0.27	0.28
DADP	0.18	0.20	0.22	0.23	0.25	0.26	0.27	0.28
PETRIN	0.33	0.34	0.36	0.37	0.39	0.40	0.40	0.42
MNX	0.11	0.14	0.16	0.18	0.20	0.22	0.23	0.25
TNX	0.08	0.10	0.12	0.15	0.16	0.18	0.20	0.21
DNX	0.10	0.13	0.15	0.17	0.19	0.20	0.22	0.23
DINA	0.24	0.26	0.28	0.30	0.31	0.32	0.34	0.35
TEGDN	0.43	0.43	0.44	0.44	0.44	0.45	0.45	0.46
HP	-0.014	-0.012	-0.01	-0.008	-0.005	-0.003	0.00	0.001
IPN	0.21	0.22	0.23	0.23	0.24	0.24	0.25	0.26
NM	0.028	0.043	0.060	0.073	0.086	0.099	0.110	0.120
ONC	0.61	0.61	0.60	0.60	0.60	0.60	0.60	0.60
TNM	0.33	0.35	0.34	0.34	0.34	0.34	0.34	0.34
TACOT	0.24	0.28	0.31	0.34	0.37	0.40	0.43	0.45
HNS	0.35	0.38	0.41	0.44	0.46	0.49	0.51	0.53
δ-HMX	-0.07	-0.02	0.03	0.07	0.11	0.14	0.16	0.18
HMTD	0.23	0.23	0.23	0.24	0.24	0.25	0.26	0.26

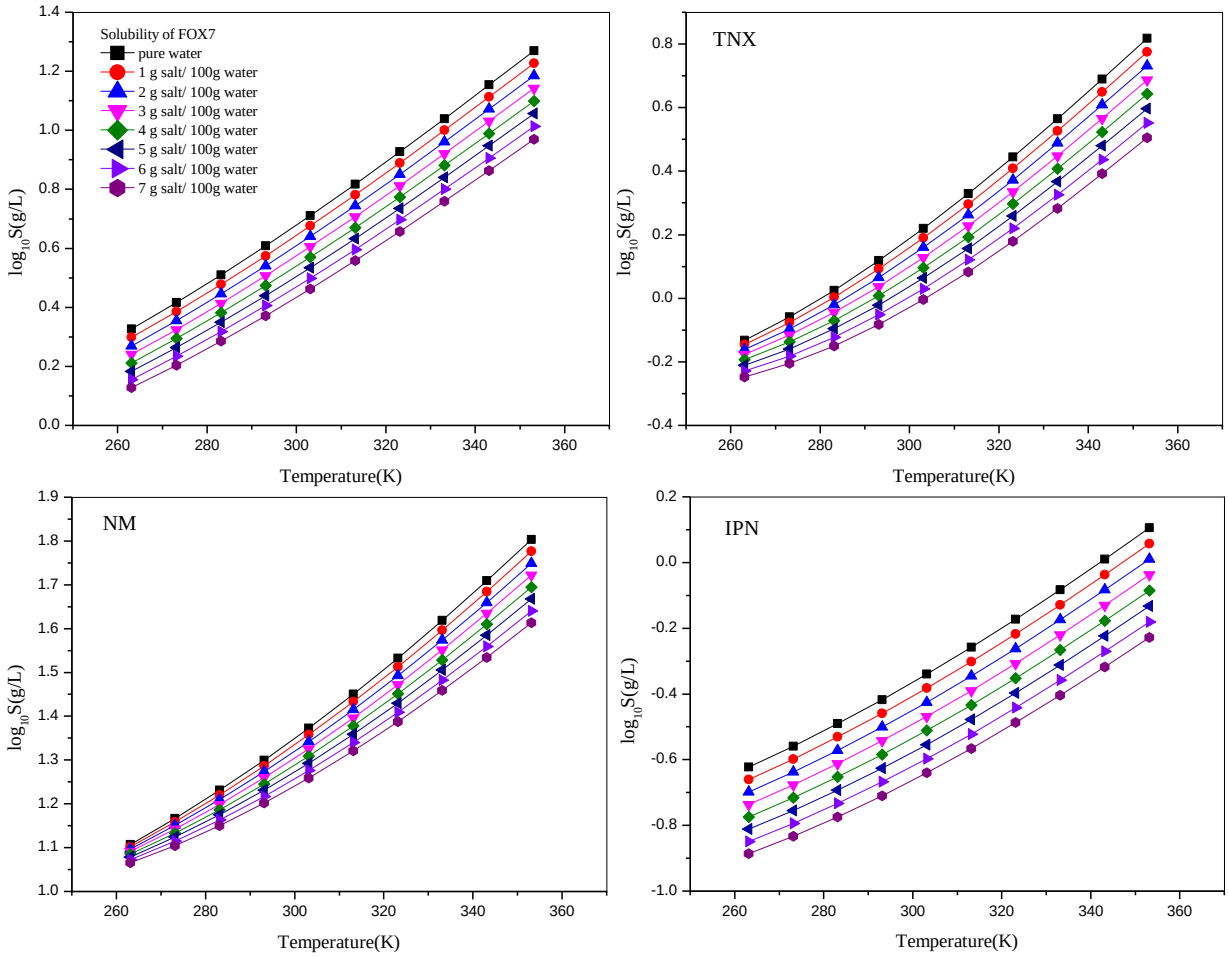

Figure S5. Higher-solubility compounds in Table S2 a function of temperature and ionic strength.

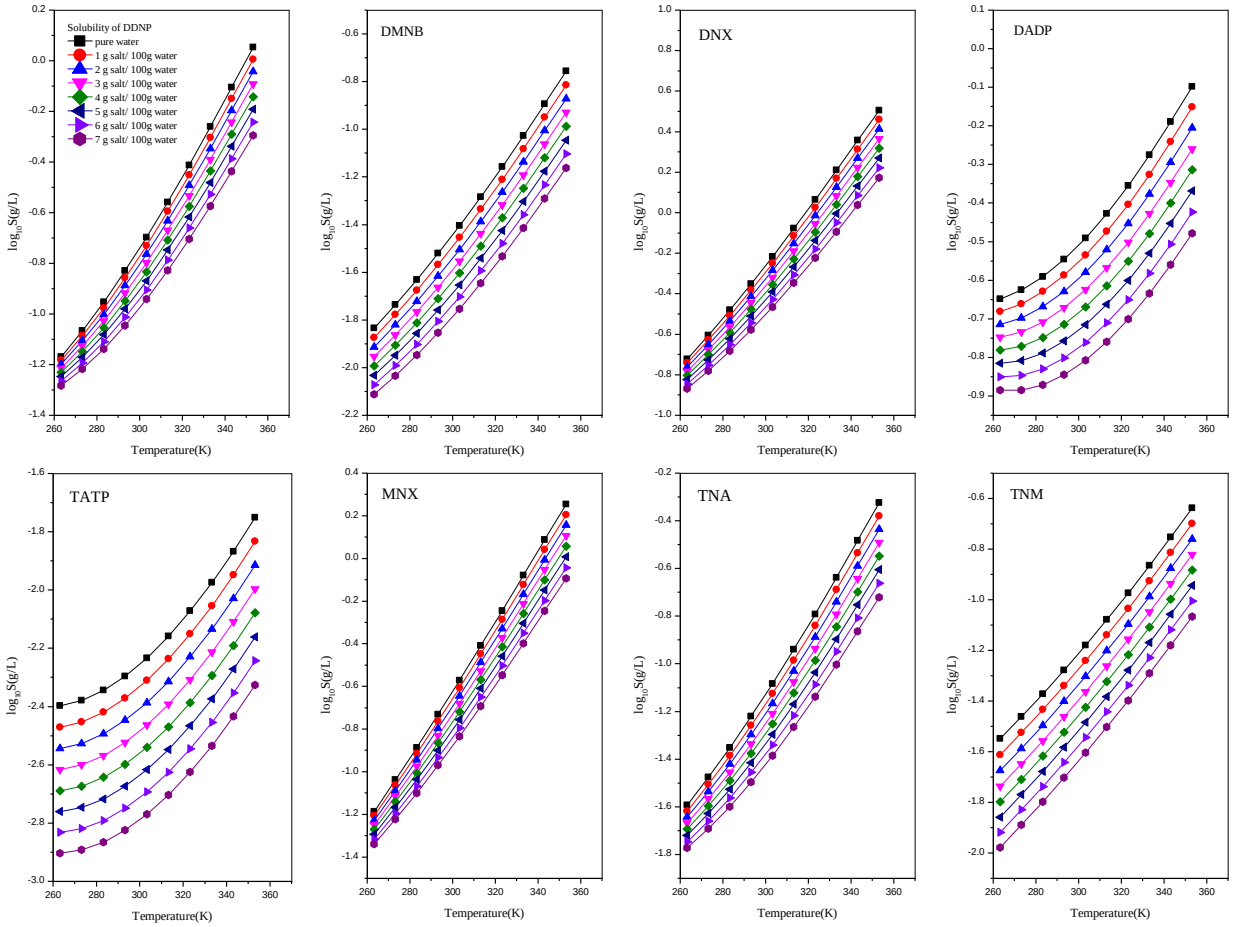

Figure S6. Intermediate-solubility compounds in Table S2 a function of temperature and ionic strength.

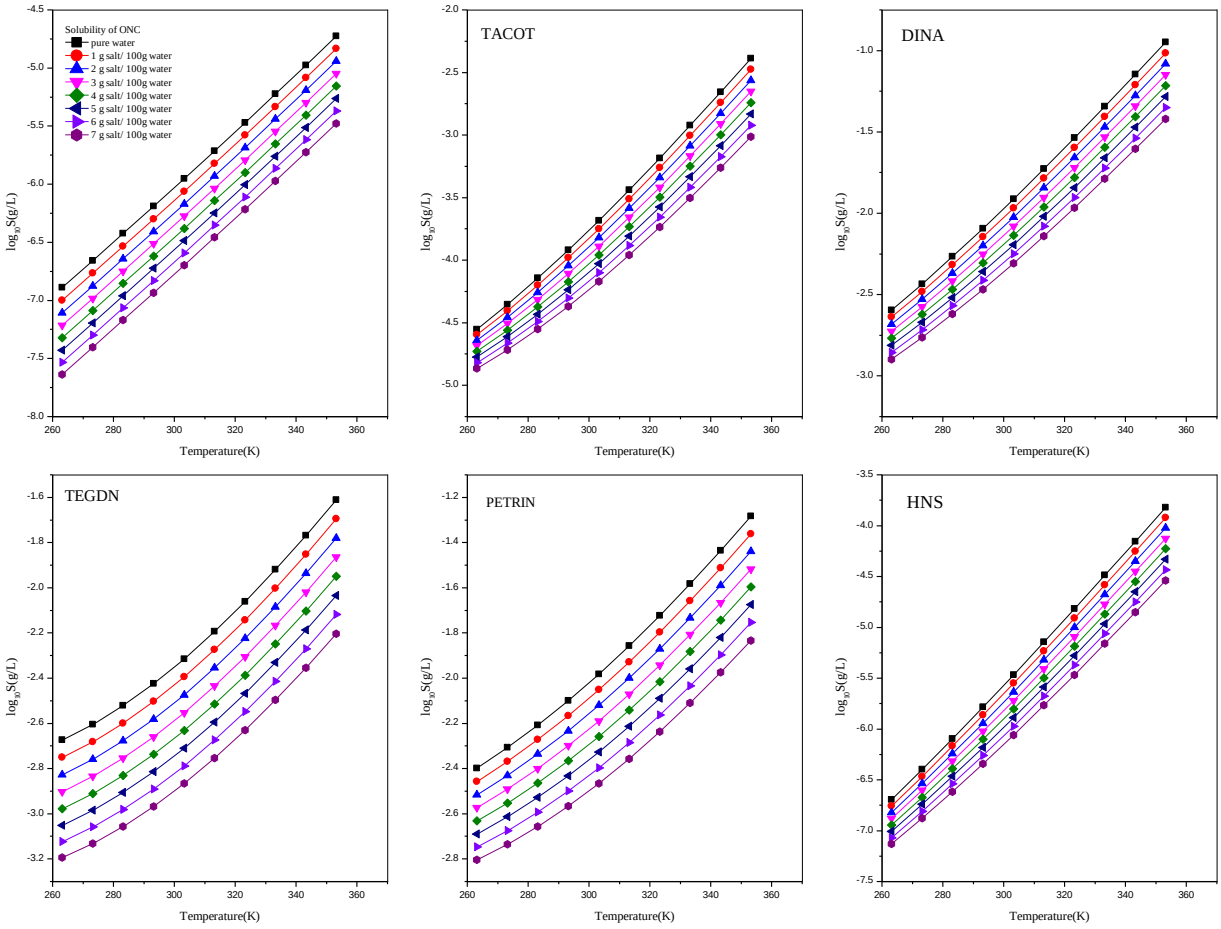

Figure S7. Low-solubility compounds in Table S2 a function of temperature and ionic strength.

Table S3. Topological parameters of representative explosives for use in estimated ΔG^{fus} values via Equation 4.

Compund	N^{rot}	N^{ring}	$V^{vdw}(A^3)$
EGDN	5	-	0.148
NG	8	-	0.216
PETN	12	-	0.301
TNT	-	6	0.224
2ADNT	-	6	0.192
4ADNT	-	6	0.192
RDX	-	6	0.210
β-HMX	-	8	0.279
TATB	-	6	0.231
CL-20	-	12	0.375